Electronic phase transitions in one-dimensional spinless fermion model with competing interactions

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An accurate numerical consideration is carried out of the ground state for the simplified model which is traditionally used for the description of Verwey transition and related phenomena. In the framework of 1D spinless fermion model, the effects of next-nearest neighbour (NNN) interaction on the metal-insulator transition are investigated for electron concentrations 1/2 and 2/3. It is shown that for large enough NNN transfer integrals the electronic topological transition of metal-metal type is also possible. The corresponding phase diagrams are presented.

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I. INTRODUCTION

Studies of highly correlated electron systems are one of the "hot" areas of condensed matter physics. A tremendous number of papers have been concerned with the problems such as heavy fermions, Mott transitions, magnetism of highly correlated systems, unconventional mechanisms of superconductivity etc. In this context the classical problem of charge ordering which has been raised by Wigner [1] and Shubin and Vonsovsky [2] (see also [3]) received far less attention. As early as the 1930s, the famous Verwey transition in magnetite Fe_3O_4 at the temperature $T_V = 120K$ has been discovered. According to the traditional views, this is the transition from the low-temperature insulating phase with Fe^{3+} and Fe^{2+} ions forming superlattice (Wigner crystal) to the high-temperature conducting phase with the destroyed charge ordering [4]. However, recent experimental data point to a more complicated physical picture since the long-range charge ordering below T_V appeared to be pronounced rather weakly [5,6] and the infrared spectra show "tunneling modes" which are presumably connected with the "smearing" of Fe^{3+} and Fe^{2+} ions over finite clusters [7]. The assertion that namely the charge ordering of Fe^{3+} and Fe^{2+} ions is the cause of the metal-insulator transition is also called in question in a number of experimental works [8,9]. Phenomena similar to the Verwey transition are observed also in a number of other compounds, e.g., in R_3X_4 (R=Sm,Eu; X=S,Se), Yb_4As_3 (see [10] and references therein), in the layered compounds RFe_2O_4 ,where R is a rare-earth ion [11]. Some of these compounds (e.g., Eu_3S_4) exhibit long-range charge ordering at low temperatures, and other ones (e.g., Sm_3Se_4) show only short-range ordering. In the latter case, a number of physical properties appeared to be anomalous, e.g., a giant low-temperature heat capacity which is not connected with current carriers is observed [12,13]. Irkhin and Katsnelson [10] suggested that an RVB (or pseudospin liquid) -type state with separated pseudospin and current degrees of freedom may be formed in such systems. Hence, the problem of description of the Verwey transition and related phenomena seems to be rather interesting from both experimental and theoretical points of view and may turn out to be closely related to the more popular areas of the physics of highly correlated electron systems.

II. THE FORMULATION OF THE MODEL

To consider the effects of strong correlations in crystals including charge ordering the polar model [2] is usually used with the Hamiltonian

$$H = -\sum_{ij\sigma}{}' t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{ij}{}' V_{ij} n_i n_j \ , \tag{1}$$

where $c^{+}_{i\sigma}$ and $c_{i\sigma}$ are the creation and annihilation electron operators, i is the site (Wannier state) index, $\sigma = \uparrow, \downarrow$ is the spin projection; $n_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}; n_i = n_{i\uparrow} + n_{i\downarrow}$ is the operator of electron number on site i; t_{ij} is the transfer integral; U, V_{ij} are the matrix elements of Coulomb interaction on-site and between different sites correspondingly, and the primed summation symbol indicates that $i \neq j$. In comparison with the original polar model this expression does not contain the multielectron contributions to the transfer processes and the direct exchange interaction (see [3]). The effects of electron-phonon interaction may be partially taken into account by the renormalization of the model parameters (e.g. the formation of small-radius bipolarons by the condition $V < 0$ etc.).

In the case of Verwey transition in the magnetite the excess electrons distinguishing a Fe^{2+} site from a Fe^{3+} one are almost completely spin-polarized ($T_V << T_C$ where $T_C = 850K$ is the Curie temperature) and fill the band by less than half. Therefore the term with $\sigma = \downarrow$ may be omitted in the Hamiltonian (1) and one may pass to the so-called spinless fermion model

$$H = -\sum_{ij}{}' t_{ij} c_i^\dagger c_j + \frac{1}{2}\sum_{ij}{}' V_{ij} n_i n_j. \qquad (2)$$

In the limit $U \to \infty$ the Hamiltonian (1) coincides with (2) [14,15]. More exactly, this is valid only in 1D case since in 2D and 3D systems the transfer Hamiltonian is renormalized by the spin-polaron effects [16]. But if we deal with ferromagnets (this is the magnetite case) the latter are absent.

The present work is devoted to the rigorous numerical investigation of the ground state of the model (2) in 1D case with the allowing for the interaction and transfer processes for the next-nearest neighbors. As it will be shown below they lead to a number of novel effects in particular to the opportunity of dimerization or electronic phase transitions of "metal-metal" type. 1D model may be considered not only as a simplified way to understand some features of real 3D case but also as a model to describe the processes in the conducting polymers and other quasi-one-dimensional crystals [17–19].

At $t_{ij} = 0$ the model (2) is equivalent to the Ising model and describes in the ground state a "frozen" electron distribution (Wigner crystal) depending on the specific form of V_{ij}. At $V_{ij} = 0$ we have the case of non-interacting electrons with the homogeneous distribution. Intuitive considerations of energy gain for competing processes show that at $t_{ij} \sim V_{ij}$ the ground state should change.

In the nearest-neighbor approximation 1D model with the Hamiltonian (2) appears to be exactly soluble [20,21]. For the electron concentration per site $\rho = 1/2$ and $V = 2$ (here and further we put $t_{i,i\pm1} = 1, t_{i,i\pm2} = t', V_{i,i\pm1} = V, V_{i,i\pm2} = V'$) the metal-insulator transition takes place with the appearance of the energy gap in the electron spectrum at $V > 2$. Let us investigate for the beginning the effect of the interaction V' on this transition at $t' = 0$.

For $t = 0$ and $\rho = 1/2$ the ground state in the model (2) is determined by the ratio of V and V' and, as it may be easily demonstrated, corresponds to the "usual" charge ordering [...10101010...] for $V' < \frac{1}{2}V$ and dimer ordering [...110011001100...] for $V' > \frac{1}{2}V$ (1 means the electron and 0 means the hole on a site). So the model (2) is frustrated because of the competing nature of the interactions V and V' (they favor different types of charge ordering).

Let us define the quantity Δ_∞ as follows: it is equal to 0 if the ground state degeneracy g is macroscopically large (i.e. increase faster than N when $N \to \infty$) at $t = 0$; otherwise it is equal to the difference between the energies of the lowest excited state and the ground one at $t = 0$. It may be shown by the direct enumeration of possible states with the same energy that at $t = 0$ the degeneracy g is exponentially large in N at $\rho = 1/2, V' = \frac{1}{2}V$ and therefore $\Delta_\infty = 0$ in this case.

One may obtain for $\rho = 1/2$

$$\Delta_\infty = \begin{cases} V - 2V' & \text{if } \frac{1}{2}V > V', \\ 2V' - V & \text{if } \frac{1}{2}V < V' < V, \\ V' & \text{if } V' > V. \end{cases} \qquad (3)$$

and for $\rho = 2/3$

$$\Delta_\infty = \begin{cases} V' & \text{if } V > V', \\ V & \text{if } V < V'. \end{cases} \qquad (4)$$

As the electron transfer is taken into account the ground state for the case $\Delta_\infty = 0$ is split into the energy band with the bandwidth of order of Nt. Since $g >> N$ this band should be continuous in the limit $N \to \infty$. Therefore one should expect that no energy gap will appear between the ground state and the lowest excited one so the ground state will be always conducting at $\Delta_\infty = 0$. At $\Delta_\infty > 0$ and $t > 0$ it is naturally to expect that the conducting ground state will transform to the insulating one with the increasing Δ_∞. The following question is to be elucidated: at what value of $\Delta_\infty^c(V, V')$ does the metal-insulator transition takes place and does the transition point depend on V and V' separately?

Hence, the following is the list of questions to be answered: (i) Does the metal-insulator transition exist at $\Delta_\infty = 0$? (ii) At $\rho = 1/2$, does the metal-insulator transition occur at $\Delta_\infty \approx 2$ similarly to the exactly soluble case $V' = 0$? (iii) More generally, do the interaction constants enter the expression for the transition point mainly via the parameter Δ_∞? (iv) How does the metal-insulator transition proceed at $\rho \neq 1/2$ in particular at $\rho = 2/3$ (this filling corresponds to the situation in many real compounds, see e.g. [10])?

These problems were considered already in a number of papers (although, to our knowledge, for the case $\rho = 1/2$ only). In [22] the phase diagram of the 1D spinless fermion model (rewritten in terms of spin operators [20]) with next-nearest-neighbor interaction has been obtained by the renormalization group approach. In [23,24] the metal and insulator regions of this model has been investigated by an exact numerical calculation of "Drude" contribution to the frequency dependent conductivity (rather general approach to the numerical calculation of correlation functions for 1D many-electron systems see e.g. also in [25,26]). However, the renormalization group method can give only general shape of the phase diagram and not the exact numerical results for the positions of phase boundaries. On the other hand, the calculations in [23] have been carried out only for few sets of parameters of the model. The recent work [24] contains the most detailed numerical investigation of the metal-insulator phase diagram in the model under consideration. Below, the problem of metal-insulator transition in the model (2) will be investigated by the calculations of the total energy and energy gap by the Lanczos method for the broader range of the parameters than in the previous papers and the answers to the

above questions will be sought for. Also the interesting phenomenon of the metal-metal transition which appears to be possible in the model with next-nearest-neighbor transfer processes will be studied.

III. METAL-INSULATOR TRANSITION: THE RESULTS OF CALCULATIONS

To investigate the ground state of the system we have used the Lanczos method of exact diagonalization for finite clusters [27,28] (really we made the calculations for $N \leq 20$) with the extrapolation to the limit $N \to \infty$. The comparison of the results with the exact ones at $t' = 0, V' = 0$ [20,21] have shown that we have at least four accurate digits in the ground state energy and two ones in the energy gap (which was calculated as the average difference of the ground state energy at the adding and removing the electron). Such accuracy is sufficient to answer the questions formulated above. The main results are the following:

1. At $\Delta_\infty = 0$ the metal-insulator transition is absent and the ground state is always metallic both for $\rho = 1/2$ and for $\rho = 2/3$ (the calculations have been carried out up to $V \sim 10^2$).

2. The metal-insulator phase diagram for $\rho = 1/2$ is shown in Fig.1. The metal-insulator transition takes place at $\Delta_\infty \approx 2$. Qualitatively this result seems rather natural. Nevertheless, it is not trivial, to our opinion, that it turned out to be valid with the accuracy comparable to the accuracy of the calculations. This result may be used for the testing of different approximations proposed for the investigation of 2D and 3D systems. Qualitatively our phase diagram is in agreement with that from [24]. Moreover, the part of the phase diagram for which real calculations has been carried out in [24] is the same. But our results for the region of large V' are new. The main difference is that, according to our results, the boundary lines of metal-insulator transition are not crossed and the metallic phase is continued to the infinity along the line $V' = V/2$ in correspondence with the qualitative discussion in the Introduction.

3. Fig.2 shows the phase diagram for $\rho = 2/3$. The criterion of the metal-insulator transition is $\Delta_\infty \approx 3$. This result is new even for the case $V' = 0$. The phase diagram for this case is qualitatively different from that for $\rho = 1/2$ (compare Figs.1 and 2). In particular, the ground state is metallic for small enough V' and *arbitrary* V. It is connected with the macroscopically large degeneracy of the ground state at $V' = 0$. Also, it is not trivial that the position of the metal-insulator boundary with the accuracy of the calculations depend only on V at $V' > V$ and only on V' at $V > V'$. Since the 1D spinless fermion model for $\rho = 2/3$ was probably not considered earlier we present in the Table 1 the results for the ground state energy and the energy gap.

4. We also have carried out the calculations for the case $\rho = 1/2$ with the adding of the third-neighbor interaction term $V'' \sum_i n_i n_{i+3}$. It appears that the criterion of the metal-insulator transition $\Delta_\infty \approx 2$ is valid also in this case provided that the interaction potential is downwards-convex namely $V + V'' > 2V'$, Δ_∞ being equal to

$$\Delta_\infty = \begin{cases} V - 2V' + 2V'' & \text{if } \frac{1}{2}(V + V'') > V', \\ 2V' - V & \text{if } \frac{1}{2}(V + V'') < V' < V, \\ V' & \text{if } V' > V, \end{cases} \quad (5)$$

This statement is illustrated by the data of the Table 2: in the case of the downwards-convex potentials (upper part of the Table) the criterion $\Delta_\infty \approx 2$ holds but no simple criterion can be established for the opposite case (lower part of the Table). Presumably, this affirmation is also valid for the electron-electron interaction of arbitrary range. The arguments justifying the downward-convexity condition for realistic quasi-one-dimensional compounds were presented by Hubbard [15].

Apart from the metal insulator transition, another interesting phenomenon studied in the spinless fermion model is the charge ordering. In particular, for $\rho = 1/2$ the interplay of "usual" and dimerized (Wigner and Peierls [22]) charge ordering can be discussed. Our approach cannot be applied directly to the solution of this problem since it is rather difficult to find asymptotics of the corresponding correlation functions directly from finite-cluster calculations. This problem can be investigated either by such approaches as analytical [22] or numerical [25] renormalization group or by the combination of exact diagonalization technique with the results of the theory of Luttinger liquid (see e.g. [26]). Nevertheless we present here our results about the characteristics of the *short-range* charge order in the model under consideration which can be interesting themselves.

The results of the calculations for the correlation functions $\langle n_0 n_1 \rangle$ and $\langle n_0 n_2 \rangle$ in the ground state for $\rho = 1/2$ are presented in Figs. 3 and 4. Consider first the case $V' < \frac{1}{2}V$. According to Fig.3 in this case we always have $\langle n_0 n_1 \rangle < \langle n_0 n_2 \rangle$ which show the absence of the dimerization. The metal-insulator transition is almost not appreciable in the calculated correlation functions describing the short-range order.

Consider now the case $V' > \frac{1}{2}V$. The data presented in Fig. 4 show that as V is decreased, the dimerized state with $\langle n_0 n_1 \rangle > \langle n_0 n_2 \rangle$ is probably destroyed before the metal-insulator transition occurs. One may suppose that as the transfer integral t is increased starting from the atomic limit, first the dimer lattice melts and then the insulator-metal transition occurs. Unfortunately the present results give us only preliminary indications of the melting of dimerized lattice (because we cannot investigate the asymptotics of the correlation functions and therefore have no direct information about long-range order), and this interesting question calls for further investigations.

The results of calculations for the correlation functions $\langle n_0 n_1 \rangle$, $\langle n_0 n_2 \rangle$ and $\langle n_0 n_3 \rangle$ for $\rho = 2/3$ and $V = 10$ is shown in Fig.5. Qualitatively the similar picture takes place for any $V' < V$. At large V and V' (or equivalently for $t \to 0$) we have $\langle n_0 n_1 \rangle \to 1/3, \langle n_0 n_2 \rangle \to 1/3, \langle n_0 n_3 \rangle \to 2/3$.

So our calculations give a rather full description of the metal-insulator transition in the 1D spinless fermion model beyond the nearest neighbor approximation. They also provide a basis for further investigations in particular concerning the relation between the metal-insulator transition and the destruction of the charge ordering. One may think that the derived conclusions about the effects of competing interactions on the nature of Verwey transition may be useful in analyzing the realistic 2D or 3D systems.

IV. ELECTRONIC TOPOLOGICAL TRANSITION IN THE MODEL WITH NEXT-NEAREST-NEIGHBOR TRANSFER PROCESSES

Apart from the metal-insulator transition considered above the interelectron interaction may lead to the electron phase transition of another type. It is connected with the next-nearest neighbor transfer processes. Although the role of such processes in many-electron models is investigated in a number of works (see e.g. recent paper [29]) the opportunity of such transition, to our knowledge, was not noted and studied.

Consider at first the case $t' \neq 0, V' = 0$. In that case at $V = 0$ one-particle electron spectrum is given by

$$\varepsilon_k = -2t \cos k - 2t' \cos 2k. \tag{6}$$

It is easily seen that at $t' > t/4$ the spectrum is nonmonotonic in the range $(0, \pi)$. At $t' > t/2$ and $\rho = 1/2$ the second fermion "pocket" appears i.e. the electron-filled region in k space is no longer singly connected. In other words, while the Fermi surface of "normal" one-dimensional system consists of two points $k = \pm k_F$ it consists of four points at $t' > t/2$ and $\rho = 1/2$. In the latter case the occupied states corresponds to the intervals $-\pi \leq k \leq -k_F^P$, $-k_F^Q \leq k \leq k_F^Q$, and $k_F^P \leq k \leq \pi$. It should be emphasized that 1D gas of non-interacting electrons cannot exhibit a dispersion low of this type since it is well known (see e.g. [30]) that the one-dimensional one-electron Schroedinger equation for a periodic potential must necessarily exhibit a monotone $E(k)$ spectrum between $k = 0$ and $k = \pi$ (the lattice parameter is set equal to unity everywhere). Nevertheless, the Hamiltonian (1) with $t' > t/4$ may be used for the description of real systems e.g. consisting of the pairs of strongly coupled one-dimensional chains with weak coupling between different pairs. In this case t is the transfer integral between the nearest sites in the direction across the double chain and t' is the transfer integral along it (see Fig. 6).

Studying of such systems is not only of purely theoretical interest. It may give a deeper insight into the properties of realistic quasi-one-dimensional systems in particular the well-known compound NMP-TCNQ (the molecules of TCNQ and NMP are shown in Figs. 7a and 7b, respectively). This compound is characterized by a charge transfer from TCNQ to NMP molecules (about 1/3 electron per NMP molecule). As one NMP-TCNQ cell contains one electron, half of the k states between $-\pi$ and π are occupied. Therefore the Fermi surface consists of two sheets: one of them is bounded by $k_F^Q = \pi/3$ and corresponds to the TCNQ chain; the other is bounded by $k_F^P = 5\pi/6$ and corresponds to NMP chain (see Fig. 7c) [17].

It is rather natural to discuss in such a case the following question: What would happen to the distribution function upon switching the electron-electron interaction, i.e., would the increasing interaction result only in a gradual smearing of the steps in the distribution function of electrons in k space or a drastic change of its shape is also possible, e.g., the merging of two steps? It will be shown below that the second possibility really takes place.

Before the presentation and discussion of exact numerical results it would be reasonable to treat this problem in the simplest Hartree-Fock approximation. The trial wave function will be chosen in the form corresponding to the distribution function with two steps in k space of the widths $2\pi\rho - 2\lambda$ and 2λ:

$$|\psi\rangle = \prod_k c_k^+ |0\rangle \tag{7}$$

where quasimomentum takes on the values $-\pi\rho + \lambda \leq k \leq \pi\rho - \lambda$ (the first step) and $-\pi \leq k \leq -\pi + \lambda, \pi - \lambda \leq k \leq \pi$ (the second step).

Substituting (7) into (2) and replacing the summation by the integration according to the formula $(1/N)\sum_k ... \to (1/2\pi)\int_{-\pi}^{\pi} dk...$ one has

$$\frac{E}{N} = \frac{\langle\psi|H|\psi\rangle}{N} = \rho^2 V - \frac{2}{\pi} t[\sin(\rho\pi - \lambda) - \sin\lambda] - \\ - \frac{1}{\pi} t'[\sin(2\rho\pi - 2\lambda) + \sin 2\lambda] - \frac{V}{\pi^2}[\sin(\rho\pi - \lambda) - \sin\lambda]^2. \tag{8}$$

In the case of $\rho = 1/2$, the substitution $x = 1 - \cos\lambda + \sin\lambda$ yields

$$\frac{E}{N} = \frac{V}{4} - \frac{2}{\pi} t + \frac{2}{\pi}(t - 2t' + \frac{V}{\pi})x + \frac{1}{\pi}(2t' - \frac{V}{\pi})x^2, \tag{9}$$

where $0 \leq x \leq 2, x = 0$ corresponds to one pocket and $x > 0$ corresponds to two pockets. Minimizing the energy with respect to x one obtains that the increase of V results in the merging of the two steps (disappearing of the second pocket) at a critical value

$$V_c = \pi(2t' - t). \tag{10}$$

This means that the switching on the electron-electron interaction, according to the usual Hartree-Fock approximation, may lead to a topological transition i.e. a change

in topology of Fermi surface: the two-sheeted (four point) "surface" transform into a one-sheeted (two-point) one. In a 3D case it would correspond to a transition from a doubly connected Fermi surface to a singly connected one which is a particular case of the electronic topological transitions proposed by Lifshitz [31]. The investigation of such opportunity by a more rigorous way is the purpose of our calculations described below.

The calculations have been carried out for a system of 10 electrons in the ring from 20 sites and of 8 electrons in the ring from 16 sites. The results for the points of the electronic topological transition in these two sets of calculations were the same with the accuracy of two significant digits. The computational results are shown in Figs. 8,9. Fig.8 displays the distribution function in the ground state $\langle n_k \rangle$ at $t' = t$. It is clearly seen that "the hump" near the edges of the Brillouin zone ($k = -\pi, \pi$) disappears at $2.5t < V < 2.6t$. Fig.9 presents the phase diagram of the system. The comparison with Eq.(10) show that beginning from approximately $t' \approx 0.8t$ the Hartree-Fock approximation gives too high values for V_c and the difference with numerical results grows with increasing t'. So, the Hartree-Fock approximation is not very accurate quantitatively at large V.

In the case $V' \neq 0$ the inverse topological transition turns out to be possible when the increase of the Coulomb interaction results in the appearance of the second pocket. We have carried out the corresponding calculations for the case $t' = 0.49t, .\rho = 1/2$. Thus, without interaction the second minimum in the electron spectrum lies very close to the Fermi level and above it. The interaction can make this minimum to be lower than the Fermi level. The phase diagram for this case is shown in Fig.10. The Hartree-Fock approximation can describe qualiatively the phenomenon of "inverse" transition but gives too high values of the critical values of V' (the difference may be in a factor of order of 2-5 depending on V values).

To conclude this section note why these results are, to our opinion, non-trivial. It is well-known that for 1D systems the electron velocity may be zero either at $k = 0$ or at the boundary of the Brillouin zone [30]. Therefore, true one-dimensional systems cannot exhibit Van Hove singularities inside the allowed band and hence they exhibit no electronic topological transitions because the latter are nothing but the crossing of the Fermi level by the Van Hove singularity. However, this is not the case for, e.g., a double chain. The exact numerical results presented here suggest that in this case quasi-one-dimensional systems do may demonstrate electronic topological transitions. As in the 3D case [31] they are, unlike metal-insulator transitions, transitions of metal-metal type. Studying the possibility of such transitions in real quasi-one-dimensional conductors containing double chains would be of experimental interest.

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[1] E.Wigner, Trans. Farad. Soc. **34**, 679 (1938)
[2] S.P.Schubin and S.W.Wonsowsky, Phys. Zs. UdSSR **7**, 292 (1935); **10**, 348 (1936)
[3] S.V.Vonsovsky and M.I.Katsnelson, J.Phys.C**12**, 2042 (1979)
[4] N.F.Mott, *Metal-Insulator Transitions* (London, Taylor and Francis, 1974)
[5] S.Iida, Phil. Mag. B**42**, 349 (1980)
[6] J.R.Cullen, Phil. Mag. B**42**, 387 (1980)
[7] P.Wachter and L.Degiorgi, Sol. State Comm. **66**, 211 (1988)
[8] K.P.Belov, Uspekhi Fiz. Nauk **163**, 53 (1993); Zh.Eksp.Teor.Fiz. **110**, 2093 (1996)
[9] A.N.Goraga et al, Zh.Eksp.Teor.Fiz. **99**, 238 (1993)
[10] V.Yu.Irkhin and M.I.Katsnelson, Pis'ma ZhETF **49**, 500 (1989); Phys. Lett. A**150**, 47 (1990)
[11] M.Tanaka et al, J. Phys. Soc. Japan **58**, 1433 (1989)
[12] T.Furuno et al, J. Magn. Magn. Mater. **76/77**, 117 (1988)
[13] O.Nakamura et al, J. Magn. Magn. Mater. **76/77**, 293 (1988)
[14] A.A.Ovchinnikov, Zh.Eksp.Teor.Fiz. **64**, 342 (1973)
[15] J.Hubbard, Phys. Rev. B**17**, 494 (1978)
[16] W.F.Brinkman and T.M.Rice, Phys. Rev. B**2**, 1324 (1970)
[17] D.Jerome and H.J.Schulz, Adv. Phys. **31**, 299 (1982)
[18] A.J.Heeger, S.Kivelson, J.R.Schrieffer and W.-P.Su, Rev. Mod. Phys. **60**, 781 (1988)
[19] J.Tsukamoto, Adv. Phys. **41**, 509 (1992)
[20] J. Des Cloizeaux and M.Gaudin, J. Math. Phys. **7**, 1384 (1966)
[21] J. Des Cloizeaux, J. Math. Phys. **7**, 2136 (1966)
[22] V.J.Emery and C.Noguera, Phys. Rev. Lett. **60**, 631, (1988)
[23] X.Zotos and P.Prelovsek, Phys. Rev. B**53**, 983 (1996)
[24] D.Poilblanc, S.Yunoki, S.Maekawa, and E.Dagotto, cond-mat/9704170
[25] H.Pang, H.Akhlaghpour, and M.Jarrell, Phys. Rev. B**53**, 5086 (1996)
[26] C.A.Hayward, D.Poilblanc and D.J.Scalapino, Phys. Rev. B**53**, R8863 (1996); C.A.Hayward and D.Poilblanc, Phys. Rev. B**53**, 11721 (1996)
[27] B.N.Parlett, *The Symmetric Eigenvalue Problem* (Englewood Cliffs, NJ, Prentice-Hall, 1980)
[28] E.Dagotto, Rev. Mod. Phys. **66**, 763 (1991)
[29] D.Duffy and A.Moreo, Phys. Rev. B**55**, R676 (1997)
[30] S.V.Vonsovsky and M.I.Katsnelson, *Quantum Solid Sate Physics* (Berlin etc, Springer, 1989)
[31] I.M.Lifshitz, Zh.Eksp.Teor.Fiz. **38**, 1569 (1960)

CAPTIONS TO FIGURES

Fig.1. Metal-insulator phase diagram at $\rho = 1/2$. Black and empty circles correspond to the metal and insulating phase, respectively; solid lines correspond to the condition $\Delta_\infty = 2$.

Fig.2. Metal-insulator phase diagram at $\rho = 2/3$. Black and empty circles correspond to the metal and insulating phase, respectively; solid lines correspond to the condition $\Delta_\infty = 3$.

Fig.3. Dependences of the correlation functions $\langle n_0 n_1 \rangle$ (circles) and $\langle n_0 n_2 \rangle$ (squares) on the parameter V for different $V' \leq V/2$: (1) $V' = 0$ (2) $V' = 0.2V$ (3) $V' = 0.3V$ (4) $V' = 0.5V$.

Fig.4. Dependence of the correlation functions $\langle n_0 n_1 \rangle$ (circles) and $\langle n_0 n_2 \rangle$ (squares) on the parameter V for $V' = 0.7V$.

Fig.5. Dependences of the correlation functions $\langle n_0 n_1 \rangle$ (circles), $\langle n_0 n_2 \rangle$ (squares) and $\langle n_0 n_3 \rangle$ (triangles) on V' at $V = 10t, \rho = 2/3$.

Fig.6. The double chain.

Fig.7. (a) TCNQ molecule (hydrogen atoms are not shown) (b) NMP molecule (c) the sketch of the dispersion law of electrons in NMP-TCNQ according to [17].

Fig.8. The distribution function $\langle n_k \rangle$ at $t' = t$. The solid line corresponds to $V = 0$, the dash-dot line corresponds to $V = 2.5t$, the dashed line corresponds to $V = 2.6t$.

Fig.9. Phase diagram of the 1D spinless fermion model at $\rho = 1/2, V' = 0$, α being the label for "one-pocket" region and β for "two-pocket" one.

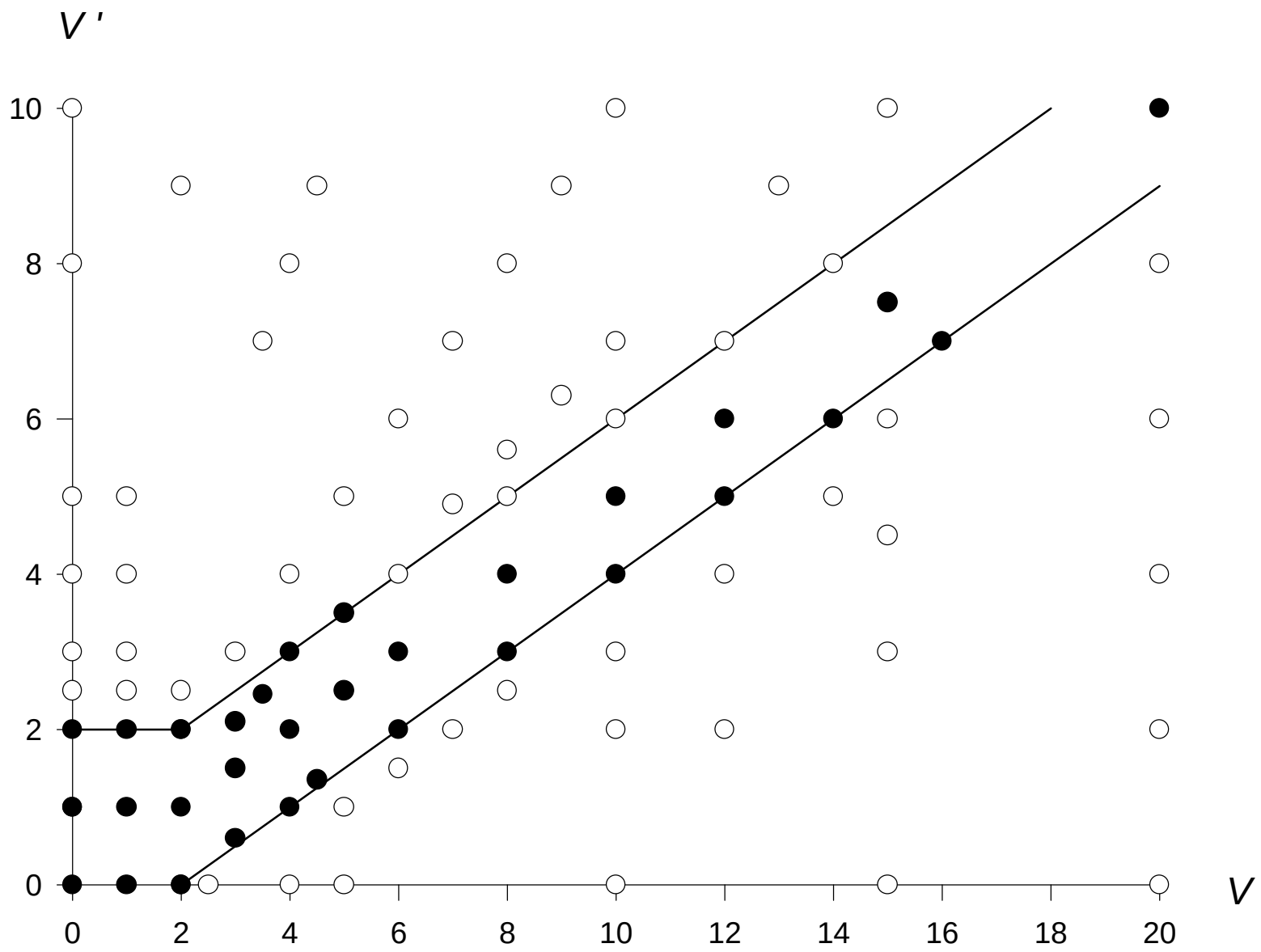
Fig.10. Phase diagram of the 1D spinless fermion model at $\rho = 1/2, t' = 0.49t$, α being the label for "one-pocket" region and β for "two-pocket" one.

TABLE II. Dependence of the gap Δ on the parameter Δ_∞ at different V, V' and V'' at $\rho = 1/2$

V	V'	V''	Δ_∞	Δ
0.5	0	0.25	1.0	0.000
2.0	1	0.50	1.0	-0.001
3.0	2	1.00	1.0	-0.001
4.5	3	1.50	1.5	0.038
1.0	0	0.50	2.0	0.003
4.0	2	1.00	2.0	0.096
6.0	4	2.00	2.0	0.180
7.5	5	2.50	2.5	0.465
1.5	0	0.75	3.0	0.263
6.0	3	1.50	3.0	0.726
9.0	6	3.00	3.0	0.873
2.0	0	1.00	4.0	1.069
8.0	4	2.00	4.0	1.827
10.0	5	2.50	5.0	3.119
3.0	0	1.50	6.0	3.335
4.0	0	2.00	8.0	5.296
2.0	2	1.00	2.0	0.002
3.0	3	1.50	3.0	0.000
4.0	4	2.00	4.0	0.156
5.0	5	2.50	5.0	1.769
6.0	6	3.00	6.0	3.494

TABLE I. Dependence of the ground state energy (the upper lines) and the gap Δ (the lower lines) on the different V and V' at $\rho = 2/3$

V'	0	1	2	3	4	5	6	8	10
V									
0	-0.5472	-0.1318	0.2662	0.6489	1.0188	1.3790	1.7324	2.4248	3.1072
	0.000	-0.001	-0.005	0.004	-0.004	-0.003	0.002	0.004	-0.001
1	-0.1856	0.2347	0.6386	1.0276	1.4031	1.7675	2.1236	2.8180	3.5016
	0.000	0.000	-0.003	0.004	0.003	0.002	0.001	0.001	-0.001
2	0.1669	0.5903	0.9984	1.3922	1.7728	2.1417	2.5010	3.1997	3.8839
	-0.001	0.000	0.000	0.002	-0.004	0.002	0.003	0.003	0.004
3	0.5135	0.9395	1.3495	1.7459	2.1292	2.5008	2.8626	3.5662	4.2545
	-0.002	0.000	0.000	-0.001	-0.004	0.005	0.005	0.005	0.006
4	0.8565	1.2832	1.6941	2.0916	2.4757	2.8467	3.2072	3.9079	4.5944
	-0.002	0.000	-0.003	0.005	0.094	0.140	0.169	0.092	0.083
5	1.1971	1.6236	2.0355	2.4332	2.8166	3.1864	3.5454	4.2440	4.9294
	-0.002	0.000	-0.001	0.020	0.309	0.610	0.876	1.018	0.932
6	1.5367	1.9631	2.3746	2.7721	3.1547	3.5234	3.8814	4.5788	5.2637
	-0.003	0.000	-0.003	0.019	0.374	1.017	1.497	1.952	1.934
7	1.8744	2.3005	2.7123	3.1095	3.4913	3.8591	4.2164	4.9131	5.5976
	-0.003	0.000	-0.004	0.039	0.422	1.316	2.042	2.803	2.925
8	2.2113	2.6376	3.0488	3.4458	3.8271	4.1941	4.5510	5.2471	5.9314
	-0.004	0.000	-0.001	0.066	0.586	1.470	2.447	3.443	3.822
10	2.8830	3.3092	3.7205	4.1166	4.4969	4.8632	5.2192	5.9147	6.5986
	-0.004	0.000	0.000	0.082	0.570	1.390	2.943	4.568	5.423
20	6.2307	6.6539	7.0639	7.4582	7.8362	8.2005	8.5555	9.2496	9.9330
	-0.004	-0.003	0.000	0.127	0.748	1.793	3.036	5.781	8.721
100	32.9074	33.3307	33.7389	34.1312	34.5074	34.8702	35.2243	35.9175	36.6004
	-0.005	-0.003	0.015	0.173	0.861	1.963	3.292	5.983	8.813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6
4
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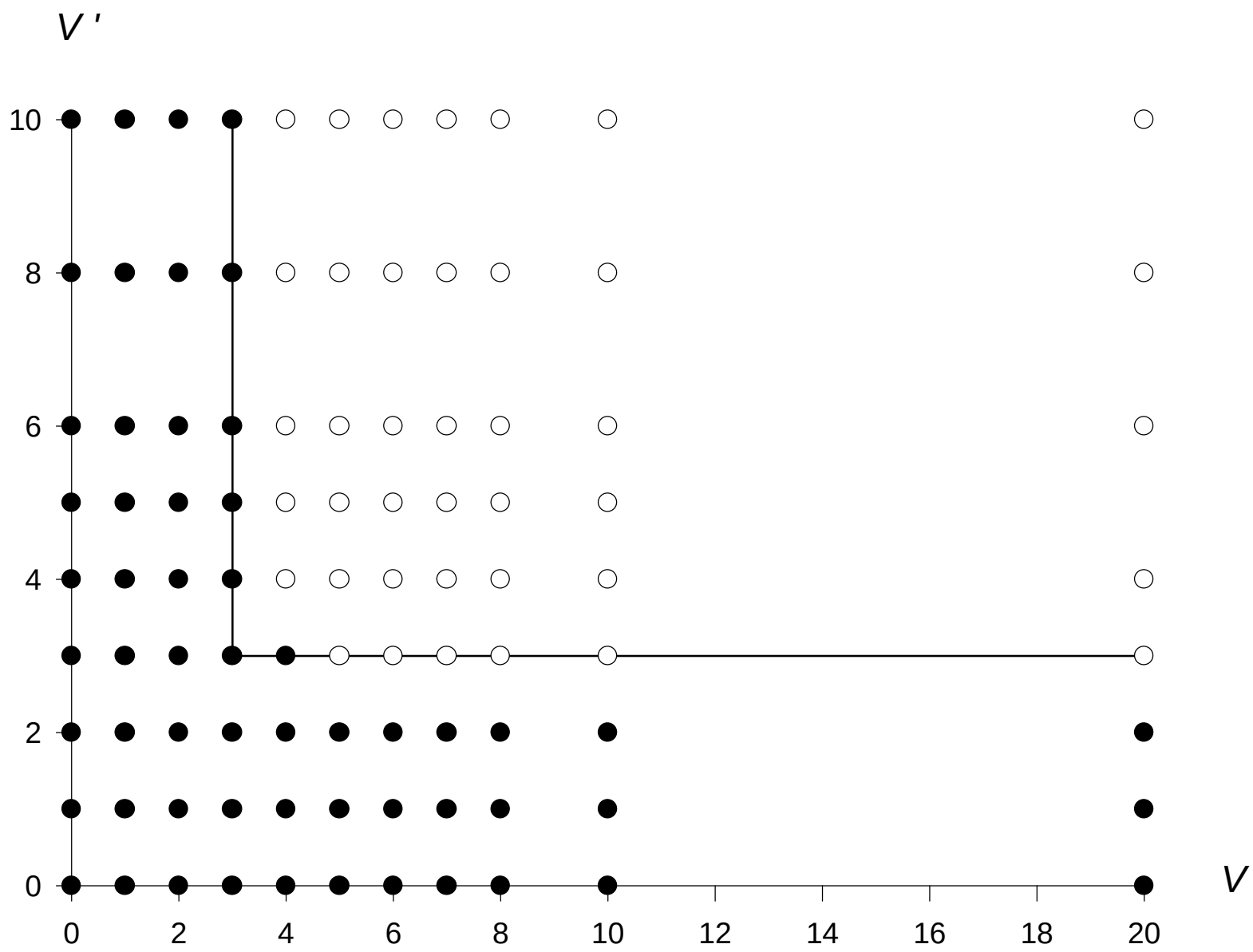
0
2
4
6
8
10
12
14
16
18
20
V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6
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2
4
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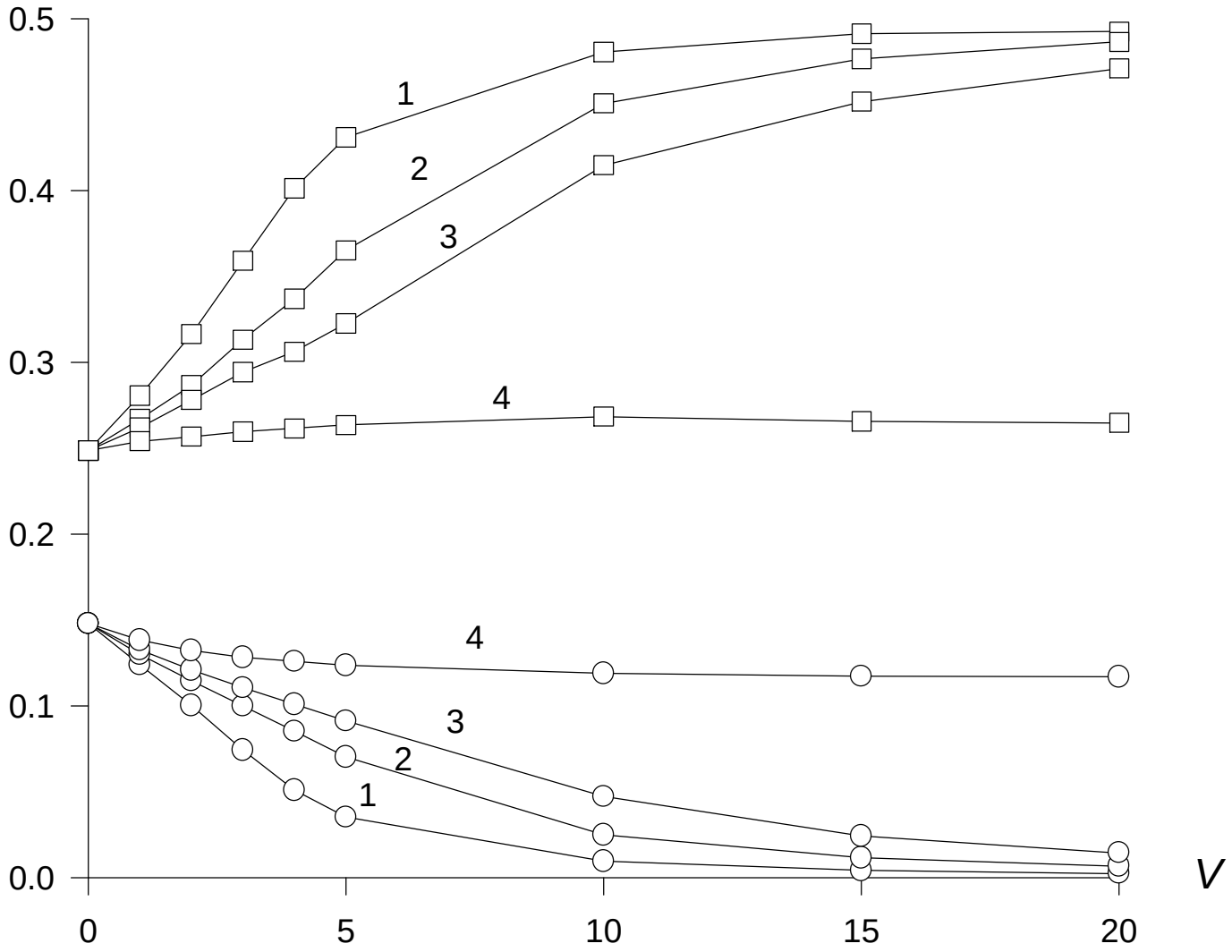
8
10
12
14
16
18
20
V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0.4
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0.2
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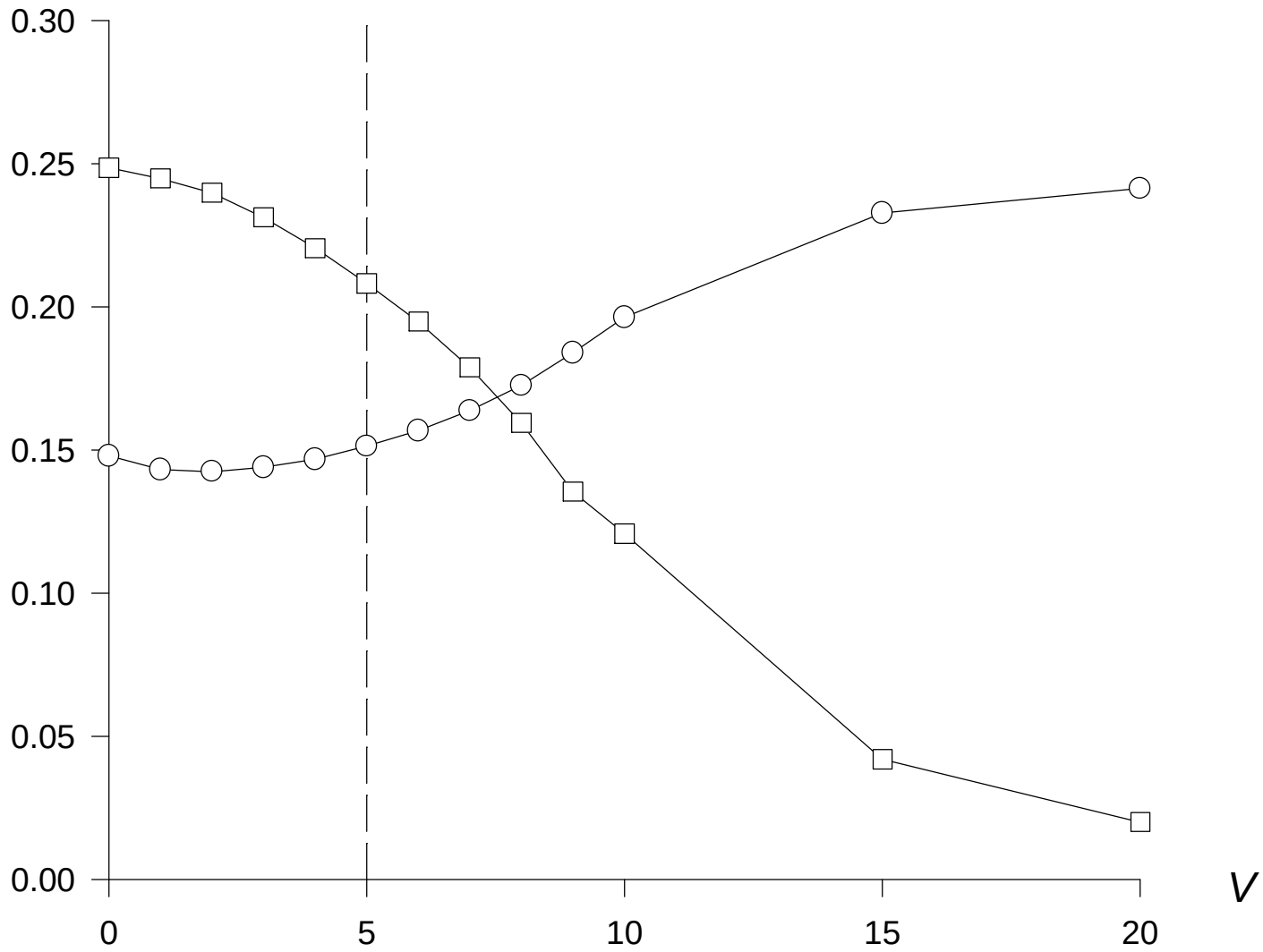
5
10
15
20
V
1
2
3
4
4
3
2
1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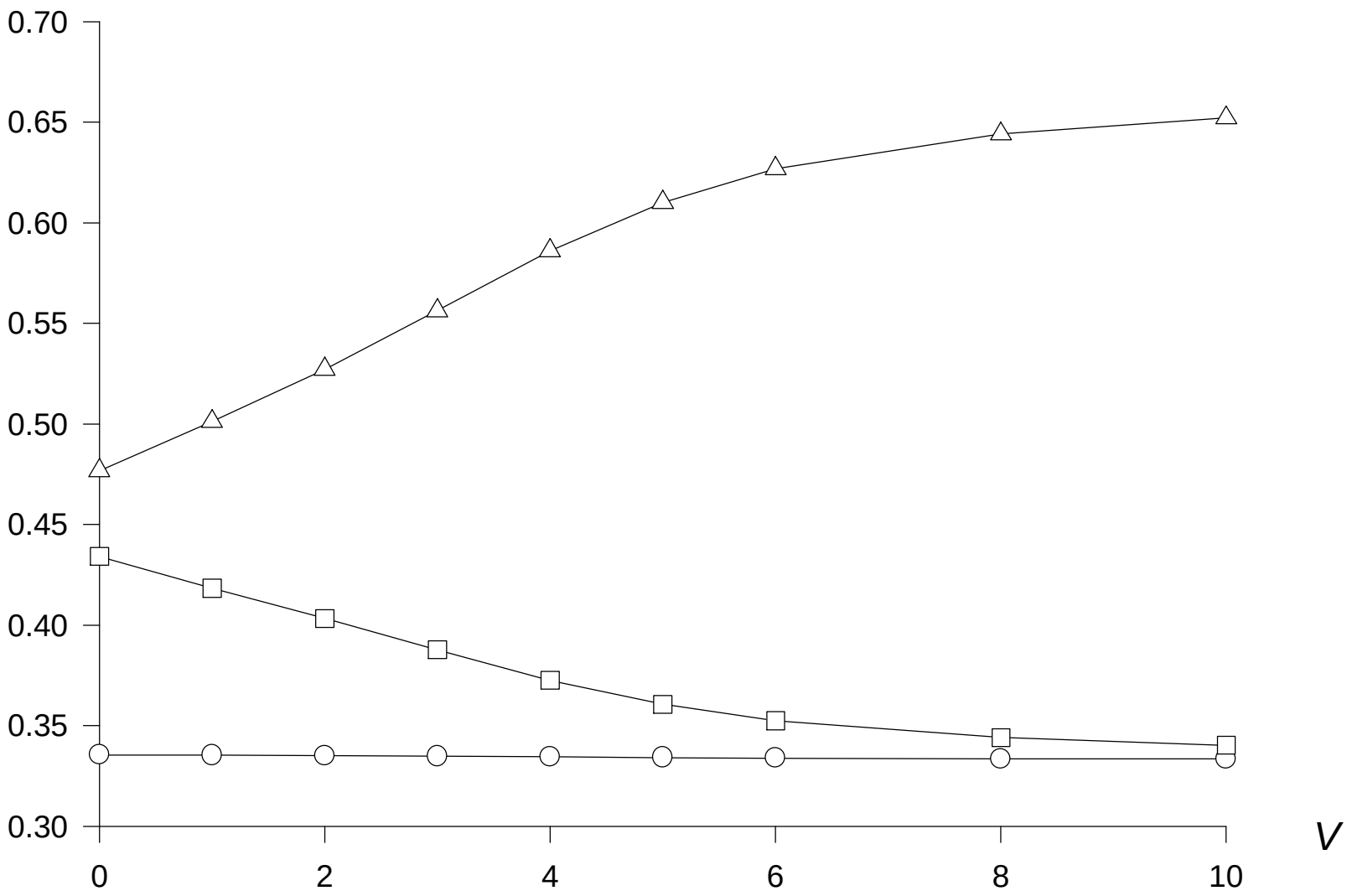
0.15
0.10
0.05
0.00
0
5
10
15
20
V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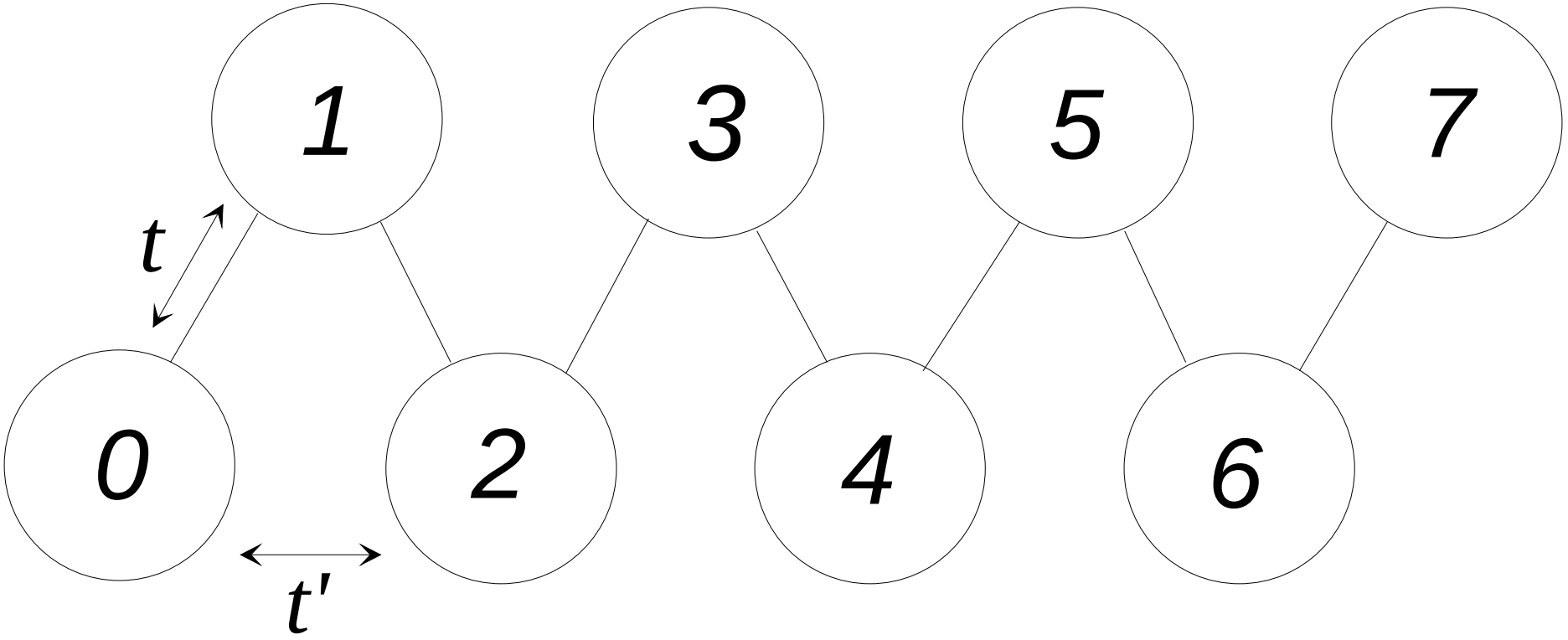
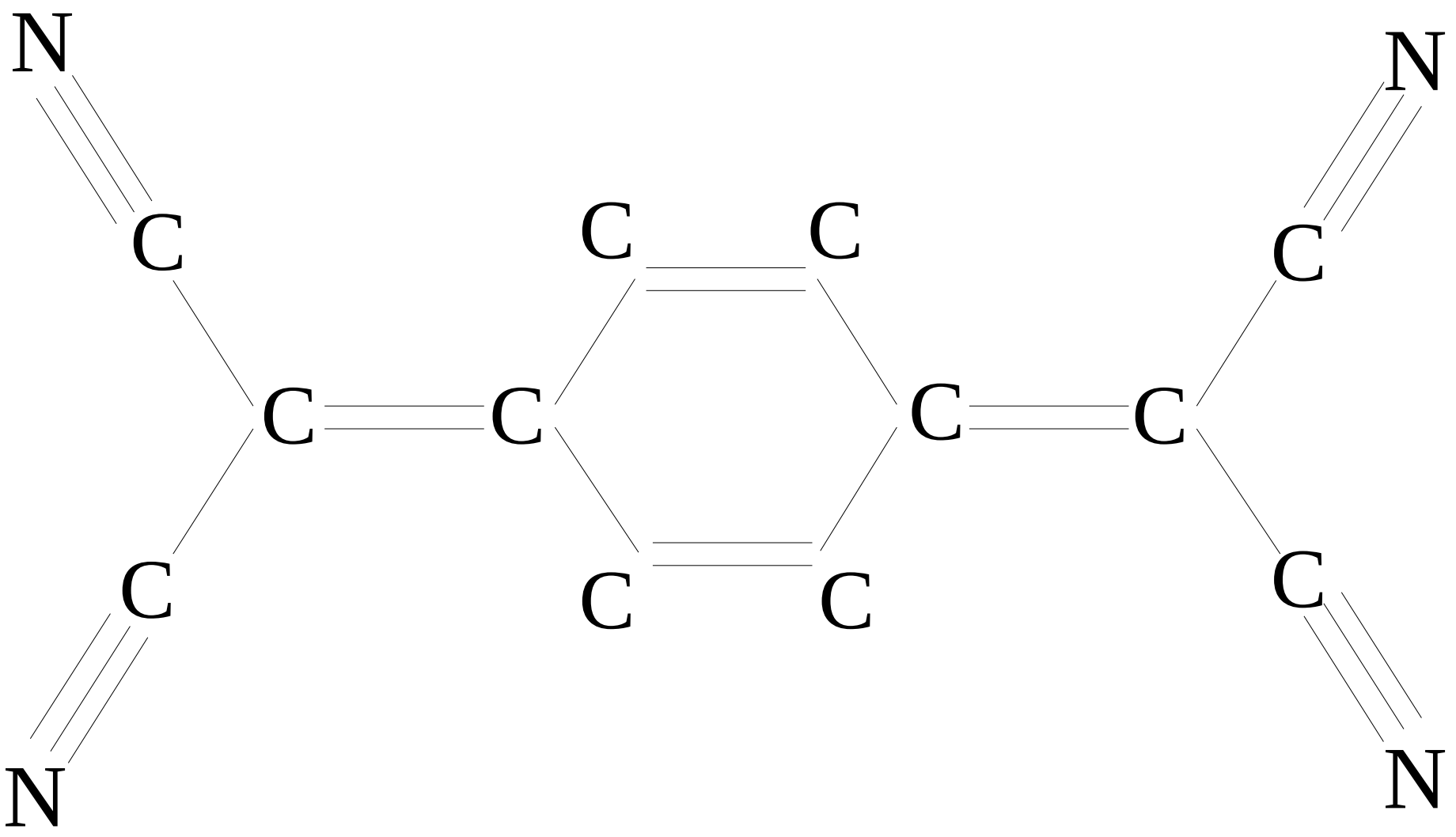
0.45
0.40
0.35
0.30
0
2
4
6
8
10
V


1
3
5
7
t
0
2
4
6
t'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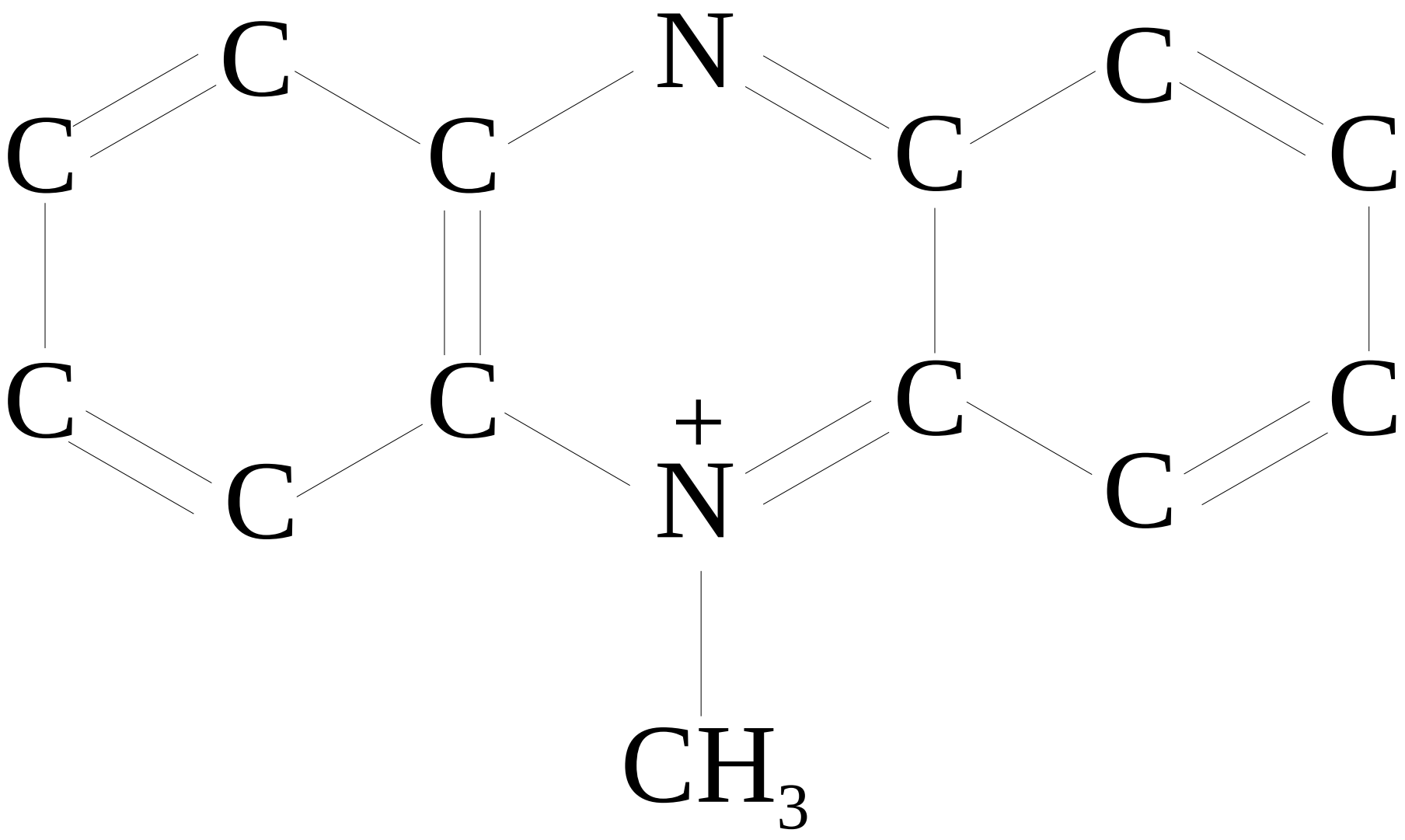
C
C
C
C
C
C
C
C
C
C
N
N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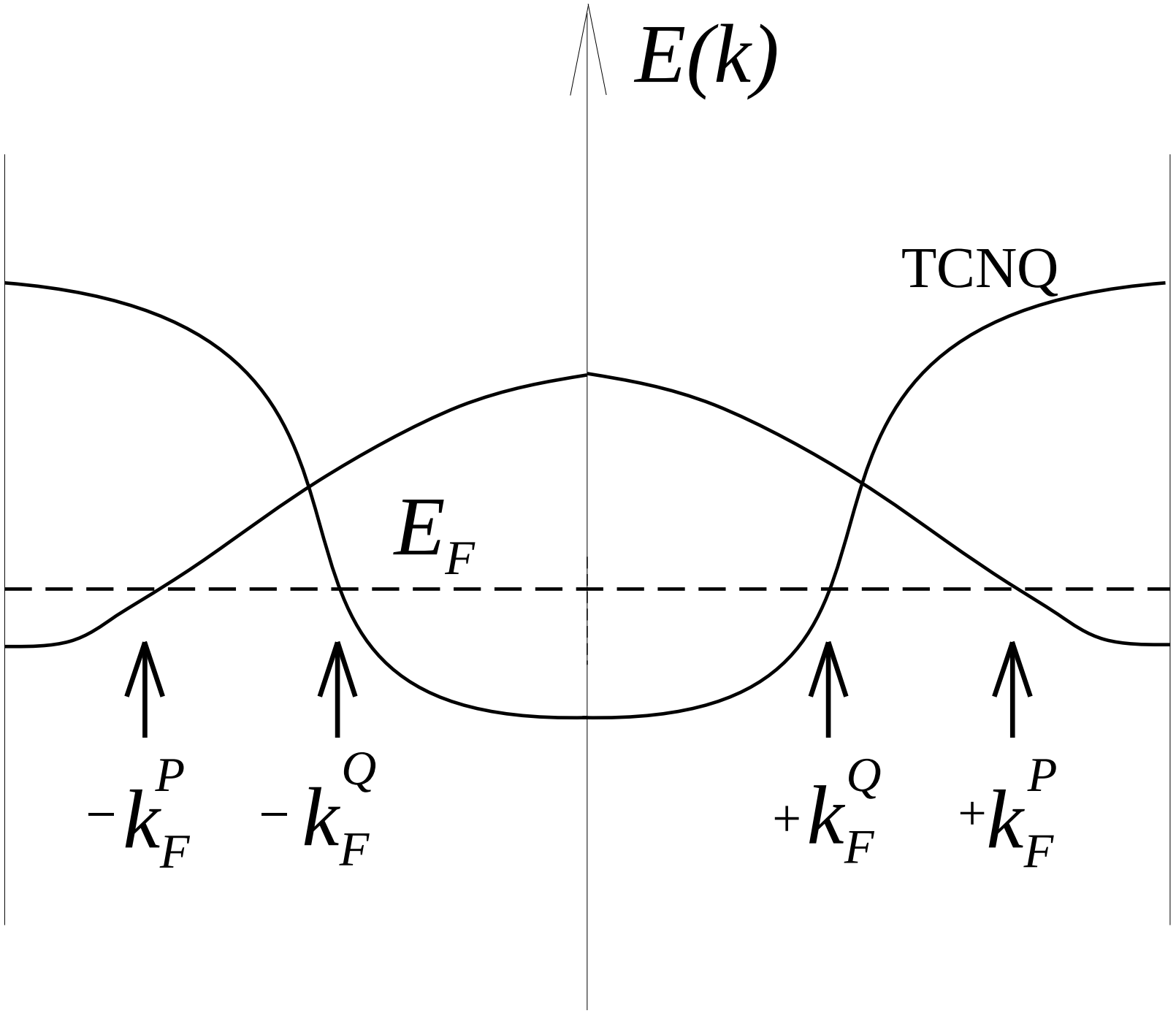
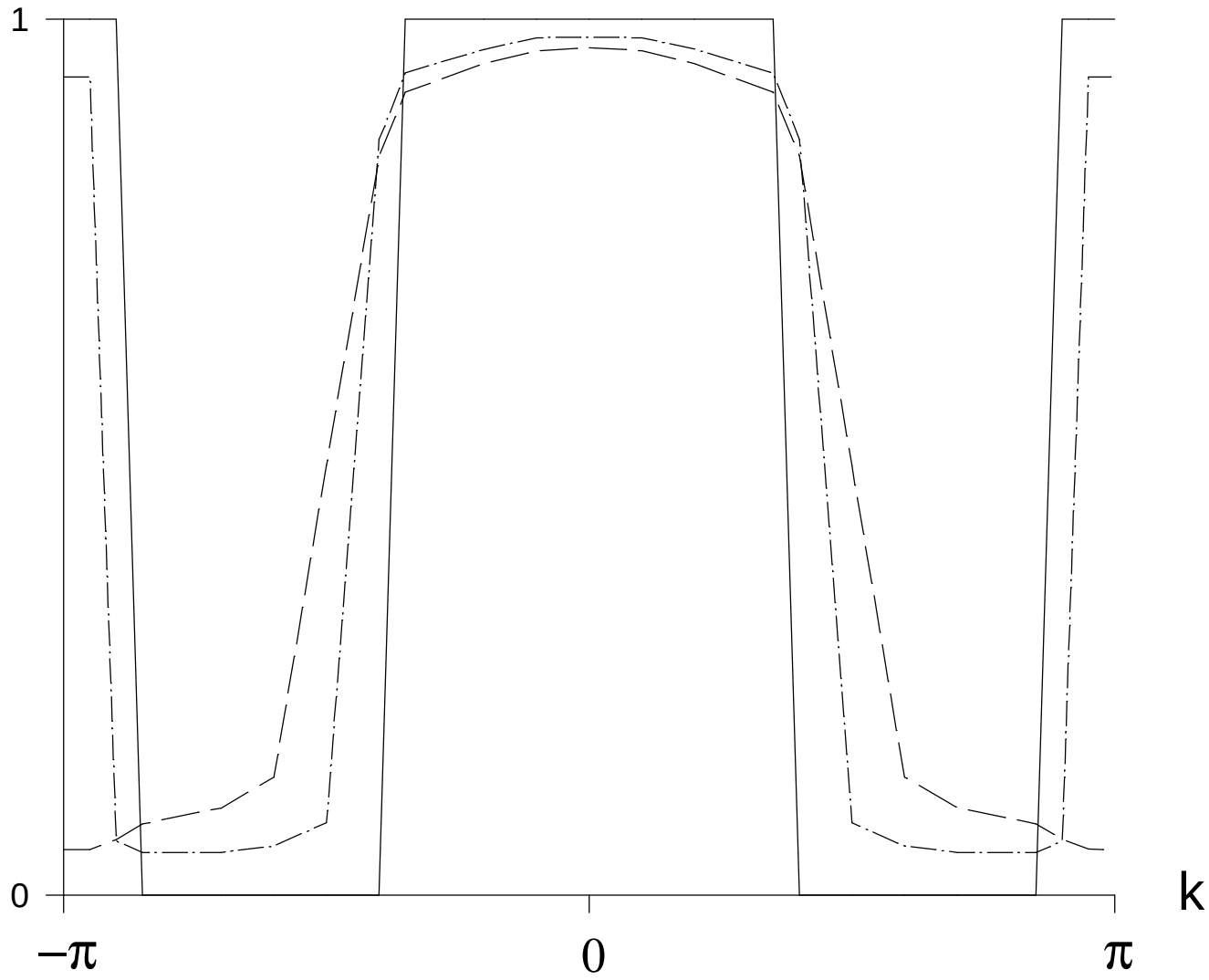
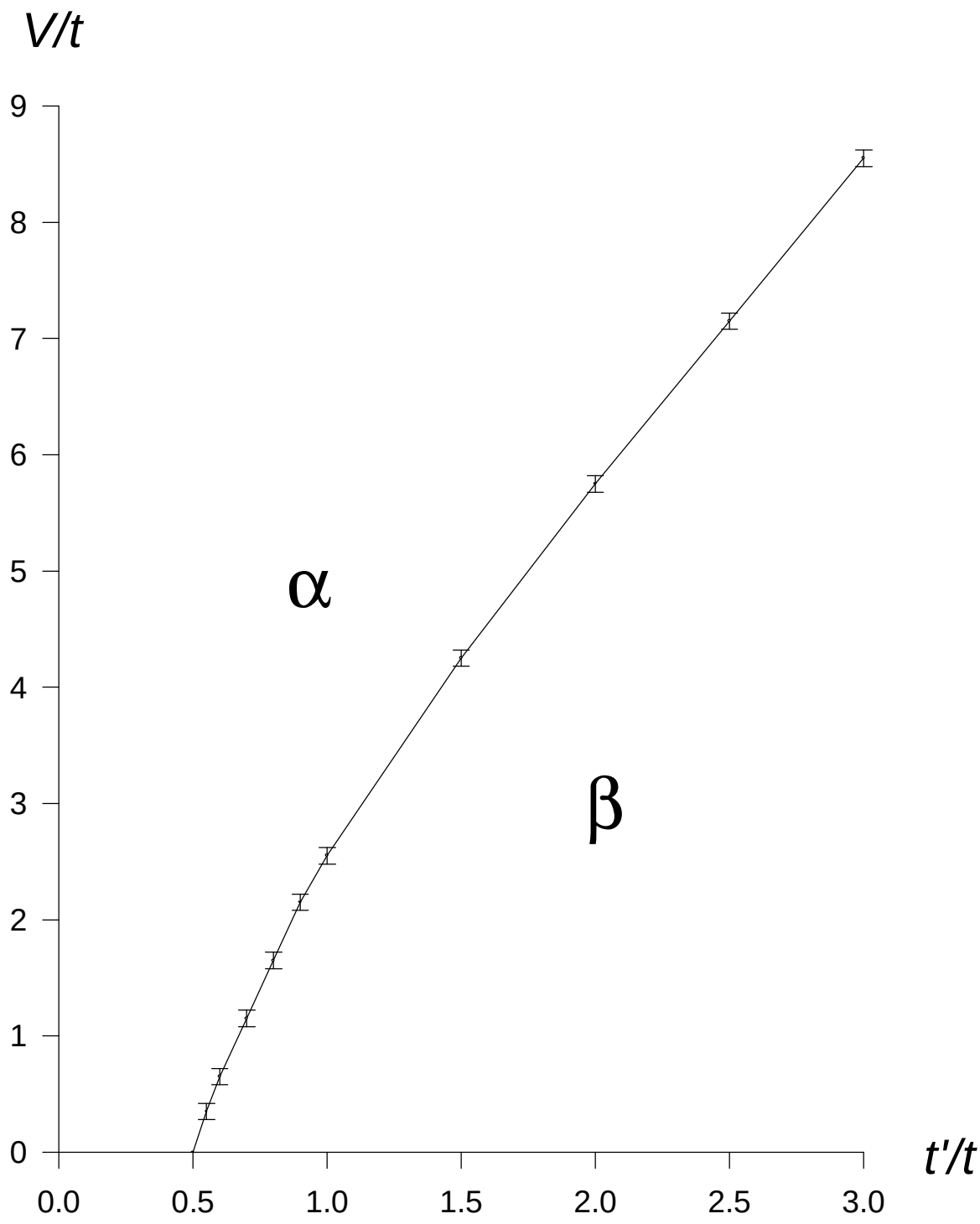
C
C
C
C
C
C
C
C
C
C
+
N
CH3


E(k)
TCNQ
E_F
$-k_F^P$
$-k_F^Q$
$+k_F^Q$
$+k_F^P$


1
0
k
−π
0
π


V/t
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8
7
6
5
4
3
2
1
0
α
β
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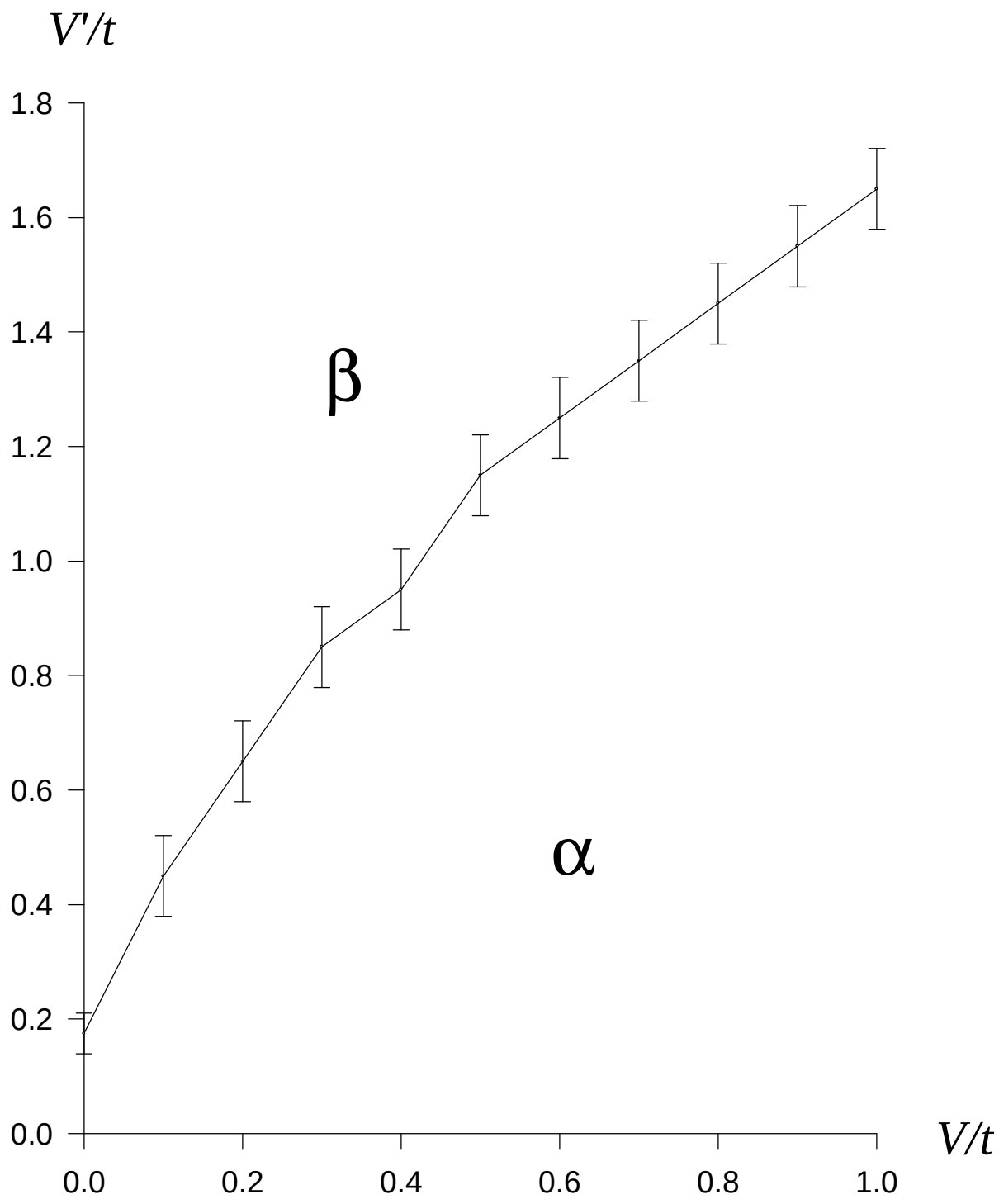
0.5
1.0
1.5
2.0
2.5
3.0
t'/t


V'/t
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1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
β
α
0.0
0.2
0.4
0.6
0.8
1.0
V/t